

Impact 5.5

User Manual

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Document Conventions

In addition to the use of italics for names of documents, the font conventions that are used in this document are summarized in the table below.

Font	Example	Use
Sans serif	Project Table	Names of GUI features, such as panels, menus, menu items, buttons, and labels
Monospace	<code>\$SCHRODINGER/maestro</code>	File names, directory names, commands, environment variables, and screen output
Italic	<i>filename</i>	Text that the user must replace with a value
Sans serif uppercase	CTRL+H	Keyboard keys

Links to other locations in the current document or to other PDF documents are colored like this: [Document Conventions](#).

In descriptions of command syntax, the following UNIX conventions are used: braces { } enclose a choice of required items, square brackets [] enclose optional items, and the bar symbol | separates items in a list from which one item must be chosen. Lines of command syntax that wrap should be interpreted as a single command.

File name, path, and environment variable syntax is generally given with the UNIX conventions. To obtain the Windows conventions, replace the forward slash / with the backslash \ in path or directory names, and replace the \$ at the beginning of an environment variable with a % at each end. For example, `$SCHRODINGER/maestro` becomes `%SCHRODINGER%\maestro`.

In this document, to *type* text means to type the required text in the specified location, and to *enter* text means to type the required text, then press the ENTER key.

References to literature sources are given in square brackets, like this: [10].

Introduction to Basic Impact

Impact is a molecular mechanics and dynamics program that provides the molecular mechanics component of Glide, Liaison, and QSite calculations. Some of the basic capabilities of Impact are also available from Maestro. These capabilities include molecular mechanics (MM) energy minimization, molecular dynamics (MD) simulations, including temperature replica exchange, hybrid Monte Carlo (HMC) simulations, and addition of explicit water solvent to a structure.

For information related to the installation and use of Impact, see the following documentation:

- The *Installation Guide*, which includes installation instructions for all Schrödinger products and documentation.
- The *Impact Command Reference Manual*, which contains syntax and keywords for Impact command input files.
- The *Maestro User Manual*, which describes how to use the features of Maestro, including the Atom Selection dialog box. An appendix describes command-line utilities, some of which may be used with Liaison.
- The *Maestro Command Reference Manual*, which contains commands, options, and arguments for running Maestro from the command line, including the Atom Specification Language (ASL) and the Entry Specification Language (ESL).

1.1 Running Schrödinger Software

To run any Schrödinger program on a UNIX platform, or start a Schrödinger job on a remote host from a UNIX platform, you must first set the SCHRODINGER environment variable to the installation directory for your Schrödinger software. To set this variable, enter the following command at a shell prompt:

```
csh/tcsh:      setenv SCHRODINGER installation-directory  
bash/ksh:      export SCHRODINGER=installation-directory
```

Once you have set the SCHRODINGER environment variable, you can start Maestro with the following command:

```
$SCHRODINGER/maestro &
```

It is usually a good idea to change to the desired working directory before starting Maestro. This directory then becomes Maestro's working directory. For more information on starting Maestro, including starting Maestro on a Windows platform, see [Section 2.1](#) of the *Maestro User Manual*.

1.2 Citing Impact in Publications

The use of this product and its components should be acknowledged in publications as:

Impact, version 5.5, Schrödinger, LLC, New York, NY, 2005.

Energy Minimization

2.1 Introduction to Basic Impact Applications

You can launch general-purpose Impact molecular mechanics calculations, called Basic Impact applications, from Maestro or from the command line, as described in [Chapter 6](#). There are four Basic Impact applications:

- Energy Minimization
- Molecular Dynamics
- Hybrid Monte Carlo
- Soak

The common features of Impact panels and Impact Energy Minimization are described in this chapter; the other three applications are described in the chapters that follow.

For an extensive set of examples of input files for Basic Impact applications, see Appendix C of the *Impact Command Reference Manual*.

2.2 Common Features of Basic Impact Panels

Maestro panels for Basic Impact applications can be opened from the Impact submenu of the Applications menu. These panels have many common features. Some features described here appear in all panels; others are common to a subset of panels.

Controls that are specific to a panel appear in the middle section of the panel. Usually the controls will be contained in a series of tabs. Each tab contains settings relevant to the task that the panel performs.

2.2.1 Source of Structure Input

Use structures from

This option menu appears in all four Basic Impact panels. The options are:

Workspace (included entry)

This is the default option. The structure that is currently included in the Workspace is used as input to the job. This includes whatever atoms, molecules, or entries are part of the structure, even atoms that have been undisplayed. Calculations with Frozen or Constrained Atoms (see

the Constraints tab, [Section 2.5 on page 13](#)) requires that you use the Workspace structure to which the constraints have been applied.

Project Table (selected entry)

Select this option to use the entry that is currently selected in the Project Table. This may be different from the structure in the Workspace. Because atom constraints are applied to the Workspace structure, they are ignored if this option is chosen.

Input for Basic Impact jobs must be a single entry in the Project Table. To use a system consisting of two or more entries as the input, choose **Merge** from the Entry menu, create a combined entry, and run the job on that entry.

2.2.2 Common Buttons

In the lower part of most panels, the following buttons appear:

Start

Click the Start button to open the Start dialog box. [Section 2.2.3](#) summarizes starting jobs using the Start dialog box.

Write

The Write button writes out all the files required for the job but does not actually start the job. Once the run files (an input file, *jobname.inp*, and one or more input structure files, *jobname_structure.mae*) are written by Maestro, the job can be run from the command line in a terminal window using the syntax:

```
$SCHRODINGER/impact -i jobname.inp
```

where *jobname.inp* is the input file for the job in question. The log output will be written to *jobname.log* by default; a different filename can be specified via *-o othername.log*.

Type `$SCHRODINGER/impact -h` for a usage summary of the `impact` command, or see [Chapter 6](#) for a discussion of running Basic Impact applications from the command line.

Close

The Close button, which is located on all Maestro panels, dismisses the current panel without starting the job or writing any files.

Help

The Help button opens your browser with an appropriate help topic displayed.

2.2.3 Starting Jobs

The features of the Start dialog box depend on the type of job which is being launched. The basic options include the following:

Output

The Start dialog box for Impact tasks includes an Output section containing one feature, the Incorporate option menu:

- **Incorporate**—Choose whether the new entries are appended to the Project Table, replace the existing entries, or are not incorporated into the Project Table at all.

Job

- **Name**—Type the name of the job in this text box, or accept the default name. When the job is started, the job name is used as the base name for files associated with the job. The Start dialog box for Impact jobs supplies an appropriate default name for each type of job (for example, `impact_soak`). However, a new default name is not automatically supplied each time you run a job of the same type. To avoid overwriting the job files from a job named `impact_soak`, use new names for the second and subsequent Soak jobs.

Note: Impact does *not* automatically assign new names to jobs or files. If files of the same name exist, a warning is displayed before any files are overwritten.

- **Host**—Choose a host, if you want to run the job on a remote machine. This option menu displays all the hosts defined in the `$SCHRODINGER/schrodinger.hosts` file, with the number of processors on the host in parentheses. The default is `localhost`.
- **Username**—Enter your user name, if it is required for running the job on remote machines. The default value is the user name of the user who started Maestro. If this user name is not correct for the selected host, you can change it in this text box. If the job is running locally, this text box is ignored.
- **CPUs**—Specify the number of CPUs to use to run the job.

Once you have finished setting these options, you can click **Start** to start the job.

2.3 The Energy Minimization Panel

The Impact Energy Minimization panel is used to set up and run an Impact energy minimization calculation on the structure in the Workspace or on an entry selected in the Project Table.

Note: *Only one entry from the Maestro Project Table can be displayed and used for each minimization job.* If you need to minimize a system that spans two entries, use the Project Table's Merge option to create a combined entry, and use that as the basis for your simulation.

To open the Impact Energy Minimization panel, choose Minimization from the Impact submenu of the Applications menu in the main window.

The Energy Minimization panel has three tabs:

- Potential
- Constraints
- Minimization

All three tabs are described in detail in this chapter. The first two tabs also appear in the Maestro panels of two other Basic Impact applications: Molecular Dynamics Simulations and Hybrid MC Simulations.

2.4 The Potential Tab

The Potential tab sets parameters that control how Impact calculates the molecular-mechanics energy in a minimization calculation or dynamics simulation. This tab is included in the Impact Minimization, Impact Molecular Dynamics, and Impact Hybrid Monte Carlo panels. The options in the Potential tab are described below.

Force field option menu

The molecular-mechanics force field to use for the calculation is chosen from this menu. Only OPLS-AA force fields are available; the options are

- OPLS_2001
- OPLS_2005 (the default)
- OPLS_2008

For calculations that use Surface Generalized Born (SGB) continuum solvation, you may want to select the OPLS_2005 or OPLS_2008 force field. With this force field, the improved parameterized nonpolar model (input file keyword `npsolv`) is used instead of the default SGB terms.

Electrostatic treatment

This option menu offers two methods for calculating the electrostatic component of the molecular mechanics energy:

- Constant dielectric

This option calculates the electrostatic interaction between atoms i and j as:

$$E_{\text{ele}} = 332.063762 \, q_i q_j / (\epsilon \, r_{ij})$$

A constant dielectric is appropriate for a vacuum (gas-phase) calculation or when an explicit or implicit solvent model is used.

- Distance dependent dielectric

This option calculates the electrostatic interaction between atoms i and j as:

$$E_{\text{ele}} = 332.063762 \, q_i q_j \epsilon \, r_{ij}^2$$

A distance-dependent dielectric is sometimes used as a primitive model for the effect of solvent. In this model, the electrostatic interaction between a pair of atoms falls off rapidly as the distance between the atoms increases. However, continuum and explicit solvent models are much better at accounting for solvent effects than a distance-dependent dielectric.

The variables in the above formulae are defined as follows:

- E_{ele} is the electrostatic interaction in kcal/mol
- q_i and q_j are the partial atomic charges on atom i and j
- r_{ij} is the distance in Å between atoms i and j
- ϵ is the Dielectric constant (see below)

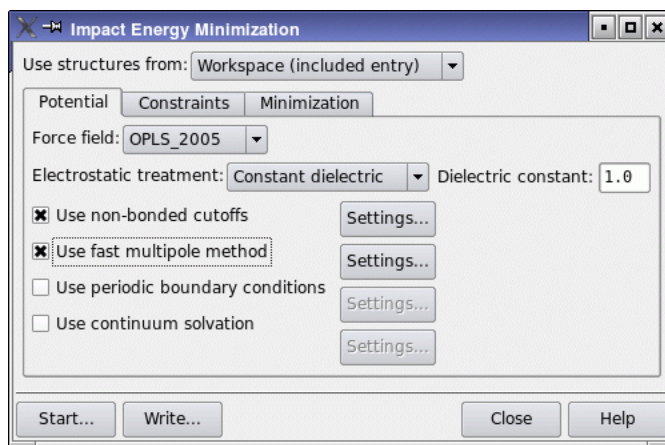


Figure 2.1. The Potential tab of the Impact Energy Minimization panel.

Dielectric constant

This text box specifies the value of the dielectric constant ϵ used in the electrostatic calculations.

2.4.1 Potential Tab Methods

The lower part of the Potential tab allows you to choose among molecular mechanics treatments. When the check box for a method is selected, clicking the associated **Settings** button opens a panel of relevant options. The methods are listed briefly in this section, and then each **Settings** panel is described in more detail.

Use non-bonded cutoffs

In molecular-mechanics calculations it is often impractical to include the nonbonded (electrostatic and van der Waals) interactions between every pair of atoms. For large systems, many such pairs are separated by a great distance and contribute little to the interaction energy. Judicious truncation of the non-bonded interactions between widely separated pairs of atoms is an important strategy for reducing the resources needed for calculations on large systems.

When this option is selected, the associated **Settings** button can be used to open the Truncation panel, from which settings for non-bonded cutoffs can be specified. The default is to use non-bonded cutoffs.

Use fast multipole method

The Fast Multipole Method (FMM) is an algorithm for speeding up the electrostatic part of the molecular mechanics calculation for large systems. It is generally used for systems without periodic boundary conditions, where Ewald summation cannot be used, and for periodic boundary explicit solvent simulations with more than 20,000 atoms.

When this option is selected, the associated **Settings** button can be used to open the Fast Multipole Method panel, from which relevant settings can be specified.

Note: The Truncated Newton (TN) minimization method and the SGB and AGB continuum solvation methods are not available for use with the Fast Multipole Method.

Use periodic boundary conditions

Periodic boundary conditions are commonly used for calculations with explicit solvent, but can be employed for any periodic system.

When this option is selected, the associated **Settings** button can be used to open the Periodic Boundary Conditions panel, from which relevant settings can be specified.

Use continuum solvation

Three implicit solvent models, Surface Generalized Born (SGB), Analytic Generalized Born (AGB), and Poisson-Boltzmann (PBF) are available in Impact. (SGB is not available if FMM has been selected.) These methods account for the effects of solvent without the use of explicit water molecules. For details on these models, see the [Impact Command Reference Manual](#).

When this option is selected, the associated Settings button can be used to open the Continuum Solvation panel, from which the choice of implicit solvation method and other settings relevant to continuum solvation can be specified.

2.4.2 The Truncation Panel

The Truncation panel defines the non-bonded cutoffs settings for an Impact calculation.

When sufficient care is taken, the use of non-bonded cutoffs to remove interactions between widely separated pairs of atoms is an important strategy for reducing the resources required to perform calculations on large systems. At present only residue-based cutoffs are supported for calculations set up in Maestro. This means that all atoms within complete residues that have any pair of atoms within the cutoff distance will be included in the non-bonded interaction list.

To open the Truncation panel, select Use non-bonded cutoffs and click the adjacent Settings button. The selection options in the Truncation panel are:

Update neighbor-list frequency (# steps) text box

When truncation is active, all the pairs that fall within the cutoff radius are stored in a “neighbor list”. During a minimization calculation or dynamics simulation, the geometry of the structure may change so as to bring some pairs of atoms that were originally outside the cutoff distance to within the cutoff. Conversely, some pairs of atoms may move outside the cutoff distance. For these reasons, the neighbor list needs to be updated from time to time. The frequency of this update is controlled by this integer field. By default the neighbor list is updated every 10 minimization or dynamics steps. Increasing this value (updating the neighbor list *less* often) will speed up the calculation but may affect the accuracy of the results. Decreasing this value (updating the neighbor list *more* often) will slow down the calculation but may improve the accuracy.

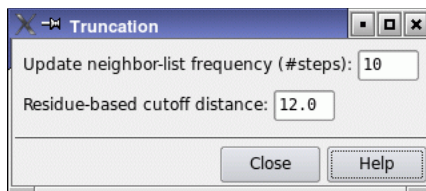


Figure 2.2. The Truncation panel.

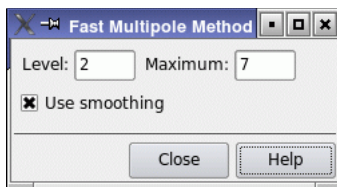


Figure 2.3. The Fast Multipole Method panel.

Residue-based cutoff distance

This text box specifies the value for the cutoff distance. Increasing the cutoff distance will slow the calculation and require more memory, but may yield more accurate results. Decreasing the cutoff will speed up the calculation, but may reduce the accuracy of the results if significant non-bonded interactions are omitted. This is especially true for systems that include formally charged atoms, as such systems can have large long-range electrostatic interactions.

2.4.3 The Fast Multipole Method Panel

For large systems, the Fast Multipole Method (FMM) speeds the evaluation of the electrostatic and van der Waals parts of the molecular-mechanics energy by using interacting hierarchical multipoles to approximate the true electrostatic potential.

In systems where long-range electrostatic effects are important, the Fast Multipole Method or Ewald summation can be used to approximate these forces. For systems of fewer than 20,000 atoms, with explicit solvent and periodic boundary conditions, Ewald summation is typically used. At about 20,000 atoms, the Fast Multipole Method becomes faster than Ewald summation: FMM calculations scale linearly with the number of atoms N , while Ewald summation scales as N^2 . FMM is also used for systems to which periodic boundary conditions cannot be applied, where Ewald summation cannot be used.

If the Fast Multipole Method is to be used with periodic boundary conditions:

- The simulation box must be a cube. Ensure that the Box [X,Y,Z] length values in the Periodic Boundary Conditions panel are equal.
- The system must be electrically neutral (the sum of all point charges must be zero).

The Fast Multipole Method cannot be used with the Truncated Newton minimization algorithm or with SGB continuum solvation.

To open the Fast Multipole Method panel, select Use fast multipole method and click the adjacent Settings button. The following options can be set:

Level

This text box sets the number of levels in the hierarchical tree used in the FMM calculation. This setting is relevant only when the reversible RESPA integrator is used with more than two inner stages. (See [Section 3.2 on page 23](#).)

The **Level** parameter specifies the number of times the simulation box is divided into halves along each direction, a procedure known as octree decomposition. If a **Level** of 1 is set, one division is made along X, one along Y, and one along Z, so that the box is divided into 8 sub-cubes (octants). If **Level**=2 (the default), each sub-cube is further divided into 8 smaller cubes, for a total of 64, and so on. The value of **Level** should be at least 2; larger values yield increased accuracy at the cost of longer execution time, but may be useful in very large systems.

Maximum

This text box sets the maximum number of multipole moments to be used to approximate the potential and field produced by “far” clusters. Currently a minimum of 4 multipoles and a maximum of 20 multipoles are permitted; the default is 7.

Use smoothing

This option, selected by default, specifies the use of a smooth cutoff to separate into “near” and “far” components the forces that are computed explicitly from Coulomb’s Law, rather than from the multipole expansions. This setting is relevant only when the reversible RESPA integrator is used with more than two inner stages. (See [Section 3.2 on page 23](#).)

2.4.4 The Periodic Boundary Conditions Panel

Impact calculations can be performed with periodic boundary conditions. This technique is usually applied with explicit solvent in order to avoid nonphysical “edge effects.” The system of interest is defined to be in a box of a given size, images of which are replicated throughout space to form an infinite 3D lattice.

The options in this panel allow you to set the size of the simulation box and to select and specify parameters for the Ewald summation method, which is used to efficiently sum long-distance electrostatic interactions in periodic systems. (This option cannot be used if you have selected **Use fast multipole method**.)

To open the Periodic Boundary Conditions panel, select **Use periodic boundary conditions**, then click the adjacent **Settings** button. The options of this panel are described below.

Box [X,Y,Z] lengths

Use these three text boxes to set the size of the simulation box. The minimum size for any dimension that Maestro will use is 18.62 Å, which is also the default in each dimension.

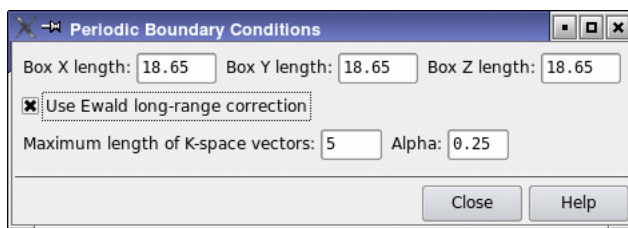


Figure 2.4. The Periodic Boundary Conditions panel.

Use Ewald long-range correction

Click to select the Ewald summation method for efficiently summing long-distance electrostatic interactions in periodic systems. Unlike the Fast Multipole Method, Ewald summation does not require the net charge of the system to be zero. This setting is ignored when the Fast Multipole Method is used.

- Maximum length of K-space vectors

If Use Ewald long-range correction is selected, you can use this text box to specify the number of component terms to retain in the reciprocal-space part of the summation. The default value is 5. Larger values yield increased accuracy but result in slower execution.

- Alpha

If Use Ewald long-range correction is selected, you can use this text box to set the value of the α parameter. A reasonable value is $5.5/L$, where L is the length of the cubic simulation box. The default value is 0.25.

2.4.5 The Continuum Solvation Panel

Impact supports three implicit solvent models, the Surface Generalized Born (SGB) model, the finite-element Poisson-Boltzmann Solver (PBF), and the Analytic Generalized Born (AGB) model. These methods simulate the effects of solvent without the use of explicit solvent molecules.

To open the Continuum Solvation panel, select Use continuum solvation and click the adjacent Settings button. The options of this panel are described below.

Solvation Method

From this option menu you can choose from the three continuum solvation models: Surface Generalized Born Model, Poisson Boltzmann Solver, and Analytic Generalized Born. If you use SGB solvation, you might want to select the OPLS_2005 or OPLS_2008 force field in the Potential tab; the improved parameterized nonpolar model (input file keyword `npsolv`) will then be used instead of the default SGB terms.

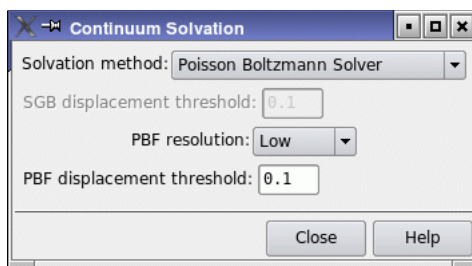


Figure 2.5. The Continuum Solvation panel.

SGB Displacement Threshold

When the Solvation method chosen is Surface Generalized Born Model, this text box specifies how far (in Å) any atom may move from the coordinates used in the previous SGB calculation before a new SGB calculation must be performed. If no atom has moved this distance, the previously calculated SGB energy and forces are used.

PBF Resolution

The Poisson-Boltzmann solver involves a finite-element calculation on a grid. The grid spacing controls both the accuracy of and time required for the PBF calculation. The default is to use a Low resolution grid, which should suffice for most protein work. If needed, greater accuracy can be achieved by setting this option menu to Medium or High.

PBF Displacement Threshold

This text box specifies how far (in Å) any atom may move from the coordinates used in the previous PBF calculation before a new PBF calculation must be performed. If no atom has moved this distance, the previously calculated PBF energy and forces are used.

2.5 The Constraints Tab

The Constraints tab of the Impact Energy Minimization panel is used to set up Impact *atom constraints*. These include constraints that freeze selected atoms at their input coordinates (frozen atoms) or keep them near their initial coordinates by applying a harmonic force (constrained atoms). Frozen atoms and constrained atoms can also be specified for Impact Molecular Dynamics (MD) and Impact Hybrid Monte Carlo (HMC) simulations, Liaison simulations, and QSite calculations, using the Constraints tabs in those panels.

The Constraints tabs in the Impact Dynamics and Impact Hybrid Monte Carlo panels can also be used to set up *bond constraints*. The MD and HMC simulations set up using these panels can use the SHAKE/RATTLE algorithm to constrain all bond lengths to ideal or reference values.

Bond constraints are not available for Impact energy minimization calculations, and the Constraints tab of the Impact Energy Minimization panel does not include bond constraint options; these options are described in [Chapter 3](#).

In the Impact and Impact Energy Minimization panels, the Constraints tab contains only two buttons: the Frozen Atoms button and the Constrained Atoms button.

Frozen Atoms

Impact calculations can be performed with some atoms completely “frozen” so that they never move from their initial position during minimization or dynamics. Click this button to open the Frozen Atoms panel, in which you can select the atoms to be treated as frozen.

Constrained Atoms

Click this button to open the Constrained Atoms panel, in which you can select the atoms to be treated as “constrained”. Constrained atoms are allowed to move, subject to harmonic penalty-function restraints that tether them elastically to their initial positions.

Note: The selection of atoms to be frozen or constrained applies only to the structure included in the Workspace when you make your selection. To apply the constraints, you must choose Workspace (included entry) as the source of structures (Use structures from option.)

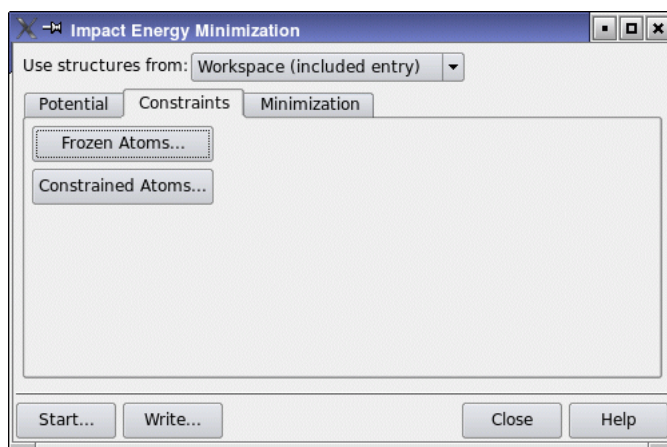


Figure 2.6. The Constraints tab of the Impact Energy Minimization panel.

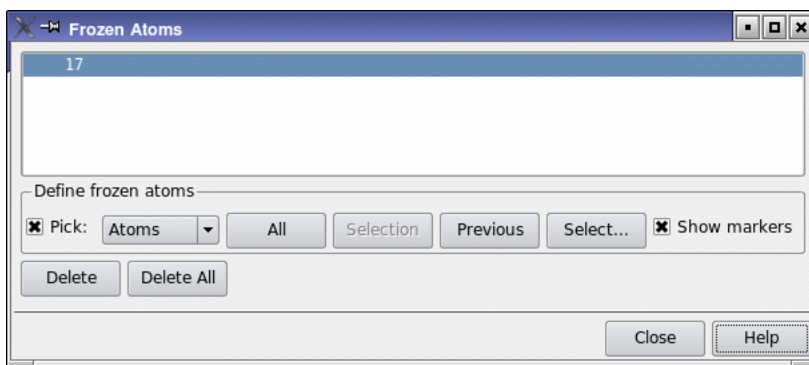


Figure 2.7. The Frozen Atoms panel.

2.5.1 The Frozen Atoms Panel

Use the Frozen Atoms panel to specify a set of atoms to be frozen during an Impact minimization calculation or dynamics simulation. Open the Frozen Atoms panel by clicking the Frozen Atoms button in the Impact Constraints tab.

The features of this panel are described below.

Frozen atoms list

The upper portion of the Frozen Atoms panel is a text area that lists the atom number of each atom that has been selected to be frozen.

Define frozen atoms

In this section you can specify atoms to be frozen using the standard picking controls: the Pick check box and menu, which is set to Atoms by default; the All button; and the Select button, which opens the Atom Selection dialog box. If you deselect the Pick check box, you can use the Workspace selection tool to select atoms, then click the Selection button to add those atoms to the list, or use the Previous button to return to the most recent selection.

Show markers option

This option is selected by default. The atoms to be frozen are marked with a red cross and a “padlock” icon in the Workspace display. To distinguish the currently selected frozen atom, Maestro colors the marker turquoise. Markers may be inconvenient if you are selecting large numbers of atoms. To prevent markers being added, or to remove the markers, deselect the option.

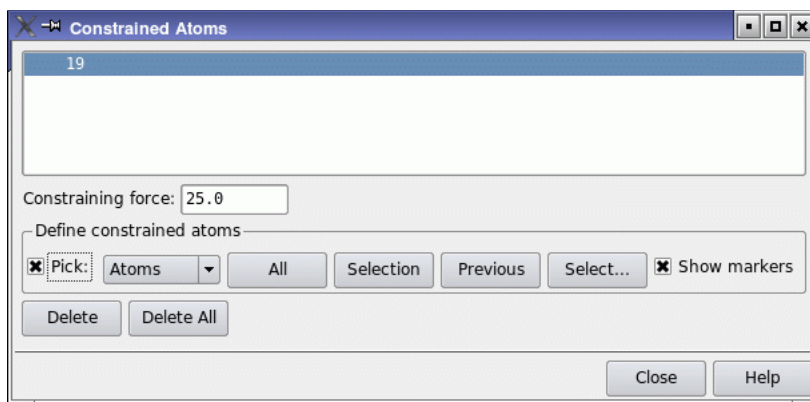


Figure 2.8. The Constrained Atoms panel.

Delete

Click this button to remove the currently selected frozen atom from the frozen atoms list.

Delete All

Click this button to remove all currently defined frozen atoms from the frozen atoms list.

2.5.2 The Constrained Atoms Panel

You can use the Constrained Atoms panel to specify a set of atoms to be harmonically restrained during a molecular mechanics calculation. Such atoms are referred to as “constrained” atoms to distinguish them from “frozen” (completely fixed) atoms. To open the Constrained Atoms panel, click the Constrained Atoms button in the Constraints tab.

Constrained atoms list

The upper part of the Constrained Atoms list displays the list of atom numbers that have been selected to be constrained (restrained with a harmonic potential).

Constraining force

This text box sets the value of the harmonic force constant applied to the selected constrained atoms. The same force constant is used for all atoms. The default is 25.00 kcal/(Å² mol).

Define constrained atoms

In this section you can specify atoms to be constrained using the standard picking controls: the Pick check box and menu, which is set to Atoms by default; the All button; and the Select button, which opens the Atom Selection dialog box. If you deselect the Pick check box, you can

use the Workspace selection tool to select atoms, then click the Selection button to add those atoms to the list, or use the Previous to return to the previous selection.

Show Markers

The Show markers option is selected by default. The atoms to be constrained are marked with a brown cross and a “spring” icon in the Workspace display. To distinguish the currently selected constrained atom, Maestro colors the marker turquoise. Markers may be inconvenient if you are selecting large numbers of atoms. To prevent markers being added, or to remove the markers, deselect the option.

Delete

Click this button to remove the selected constrained atom from the constrained atoms list.

Delete All

Click this button to remove all defined constrained atoms from the constrained atoms list.

2.6 The Minimization Tab

The basic settings of the Impact energy minimization task are defined in the Minimization tab. You can use this tab to set options for an Impact energy minimization calculation on the structure specified in the Use structures from option menu in the Impact Energy Minimization panel. The Impact Minimization tab is available in the Impact Energy Minimization panel.

Note: In Liaison, minimization options for simulations are available in the Parameters tab.

The options available in this tab are described below.

Maximum minimization cycles

This text box sets the maximum number of cycles for the minimization calculation. The minimization terminates if it has not converged by this point. The default value of this setting is 100 iterations, but you can specify any value greater than or equal to zero. “Zero cycles” is a special case; it instructs Impact just to evaluate the energy for the current coordinates.

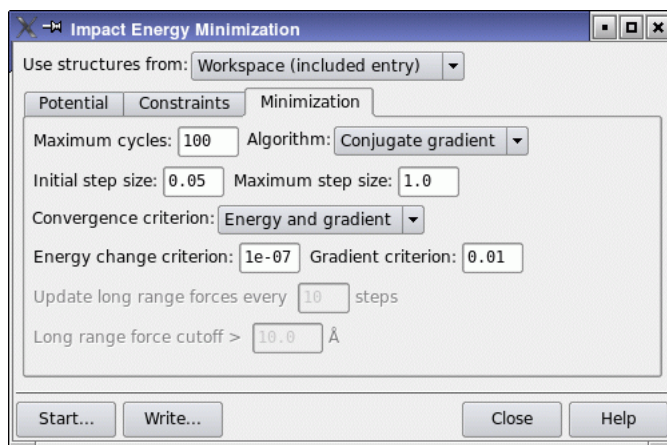


Figure 2.9. The Minimization tab of the Impact Energy Minimization panel.

Algorithm

This option menu selects the minimization algorithm. The choices are:

- Truncated Newton (TN). This is a very efficient method for producing optimized structures and is the current default selection. A short conjugate gradient pre-minimization stage is performed first to help improve the convergence of the Truncated Newton algorithm.
 - The Truncated Newton minimization algorithm is not available if Use fast multipole method (FMM) has been selected in the Potential tab.
 - The Truncated Newton minimization algorithm is only available with the generalized Born (SGB and AGB) continuum solvation methods. It is not available with explicit solvent models, such as set up in the Soak panel.
- Conjugate gradient. This is a good general optimization method.
- Steepest descent. This can be a good method for initiating a minimization on a starting geometry that contains large steric clashes. Convergence is very poor towards the end of minimization, where the conjugate gradient algorithm should be used.

Initial step size

This text box specifies the initial step size of the minimization cycle for conjugate gradient and steepest descent minimizations. The default value is 0.05 Å, but any positive value is allowed.

Maximum step size

This text box specifies the maximum step size of the minimization cycle for conjugate gradient and steepest descent minimizations. If the step size exceeds this value, the minimization will halt. The default value is 1.00 Å, but any positive value is allowed. The maximum step size is the maximum displacement allowed for an atom in any step of a minimization calculation.

Convergence criteria

This option menu sets the convergence criteria for the minimization. Either or both of two criteria—energy change and gradient—can be specified. Thus, the options are:

- **Energy and Gradient.** Choosing this option allows access to both the Energy change criteria and Gradient criteria text boxes.
- **Energy change criteria.** Use this text box to specify the value of the energy change criterion. The default value is 10^{-7} kcal/mol, but any positive value is allowed. The criterion is applied to the average energy per atom, and is satisfied if two successive average energies differ by less than the specified value.
- **Gradient criteria.** Use this text box to specify the value of the gradient criterion. The default value is 0.01 kcal/(mol*Å), but any positive value is allowed. The criterion is satisfied if the norms of two successive gradients differ by less than the specified value.

Long-range forces options (for Truncated Newton minimizations):

- **Update long range forces every n steps.** Use this text box, when Truncated Newton minimization is selected, to specify the frequency with which long range forces are updated. Between these intervals, estimates of these forces are used. Every 10 steps is the default; smaller numbers (more frequent updates) can be used to improve convergence, but will make the optimization slower. Larger numbers for n may speed the calculation, but the maximum recommended value is 20.
- **Long range force cutoff $> d$ Angstroms.** Use this text box, when Truncated Newton minimization is selected, to specify the distance beyond which forces are considered long range and are therefore updated every n steps. The default value is 10.000 Å.

Molecular Dynamics Simulations

You can use the Dynamics panel to set up and run a Molecular Dynamics (MD) simulation on the Workspace structure. Molecular Dynamics simulations examine stable, ground state molecules by applying Newton's equations of motion. The constant volume and temperature (NVT) ensemble is the default ensemble for MD simulations. The constant volume and energy (NVE) and constant pressure and temperature (NPT) ensembles are also supported, as is temperature replica exchange.

NPT simulations require the use of periodic boundary conditions (see [Section 2.4.4 on page 11](#)). Such calculations often, but not always, use explicit solvent (see [Chapter 5](#)).

To open the Dynamics panel, choose Dynamics from the Impact submenu of the Maestro Applications menu. The Dynamics panel has the following tabs:

- Potential
- Constraints
- MD Parameters
- Dynamics
- Replica Exchange

The Potential and Constraints tabs are described in [Chapter 2](#). The Constraints tab in the Dynamics panel includes features not available for energy minimization or Impact. These features are described here, along with the MD Parameters tab, and the Dynamics tab, and the Replica Exchange tab.

When you have set the options in the Dynamics panel tabs to the desired value, click the Start button to open the Impact Dynamics - Start dialog box. The standard job start options are displayed, including the Incorporate option menu and the Job options: Name, Host machine, and Username (if different from the user name on the local host). For a description of these options, see [Section 2.2.3 on page 5](#). The default job name for Impact Molecular Dynamics jobs is `impact_dyn`.

The input for an Impact Molecular Dynamics job can be either the contents of the Workspace or a single entry in the Project Table.

Note: *Only one entry from the Maestro Project Table can be displayed and used for each dynamics job.* If you need to merge two entries, use the Project Table's Merge option to create a combination entry, and use that as the basis for your simulation.

3.1 The Constraints Tab

In addition to the features described in [Section 2.5 on page 13](#), the following features appear in the Constraints tab in the Impact Dynamics and HMC calculations:

Constrain all bonds

When this option is selected, all bond distances are constrained to their “ideal” values as defined by the molecular force field, using SHAKE to constrain the bond length and RATTLE to remove the relative motion (velocity) of the bonded atoms along the interatomic axis.

By default, Constrain all bonds is selected in the Impact Dynamics panel, but not selected in the Impact Hybrid Monte Carlo panel.

Make water molecules rigid

When this option is selected, the internal coordinates of water molecules are constrained to their “ideal” values as defined by the molecular force field. If you select Constrain all bonds, the HO distances are fixed but the HOH angles are not. This option adds the HH distances and the HO distances to the SHAKE distance constraints list, so that the water molecules become rigid. (The HO distances are not added if they are already in the list).

By default, Make water molecules rigid is selected in the Impact Dynamics panel, but not selected in the Impact Hybrid Monte Carlo panel.

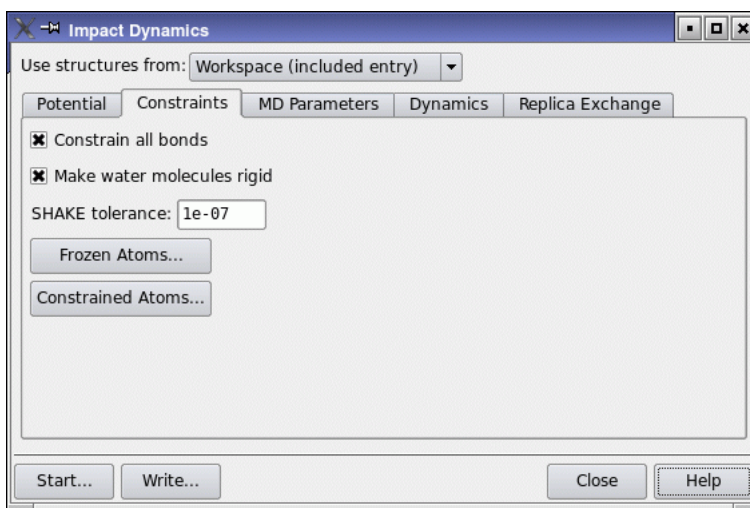


Figure 3.1. The Constraints tab of the Impact Dynamics panel.

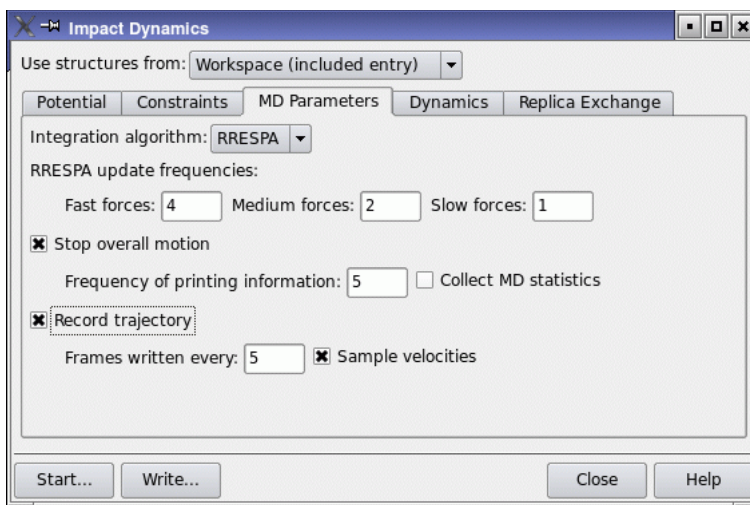


Figure 3.2. The MD Parameters tab of the Impact Dynamics panel.

SHAKE tolerance

This text box sets the tolerance for the SHAKE/RATTLE algorithm. The default value is 10^{-7} Å for SHAKE and 10^{-7} Å/ps for RATTLE. Increasing the tolerance will speed the calculation at the cost of allowing greater variation from the ideal values. Any value greater than zero is allowed. Note that the same numeric value is used for both tolerances, even though the units are different.

3.2 The MD Parameters Tab

In the MD Parameters tab you can specify molecular dynamics settings that affect both Molecular Dynamics (MD) and Hybrid Monte Carlo (HMC) calculations (see [Chapter 4](#)). The options are described below.

Integration algorithm

This option menu specifies the integration algorithm employed to integrate the Equations of Motion (EOM). The options are Verlet and RRESPA. There are no other settings to specify for the Verlet option. When RRESPA is selected, three other text boxes become active, as noted below.

- Verlet. The widely used velocity Verlet integration algorithm is the default for integrating the equations of motion in standard Cartesian-space molecular dynamics.

- **RRESPA.** The Reversible REference System Propagator Algorithm), the other choice offered by Impact for integrating the EOM, can be much more efficient. By breaking up the integration into large, medium, and small time steps (see the RRESPA update frequencies text boxes), this integrator devotes appropriate computational power to specific classes of forces—and thus keeps the calculation from being dominated by the small time steps needed to accurately integrate the fast motions (such as bond stretches). In particular, RRESPA integrates the fast motions with small time steps and the slow motions (far more numerous) with larger time steps.
- **RRESPA update frequencies.** If you select RRESPA, text boxes for Fast forces, Medium forces, and Slow forces are enabled.

When the Fast Multipole Method (FMM) is also used, the forces are separated into three groups: those arising from well-separated bodies, those arising from first and second neighbors that are not very close, and those coming from the local expansions, which include bonded terms.

Table 3.1. RRESPA text boxes

Force	Interacting Species	Default Setting
Fast	Bonded and short-distance electrostatics	4
Medium	1 st and 2 nd neighbors that are not close	2
Slow	Long-distance non-bonded	1

All text boxes have acceptable ranges of any integer value greater than one. These entries modify the time step for the underlying MD or HMC simulation in the following way. Suppose that the global Time step specified in the Dynamics tab of the Impact Dynamics panel or the Hybrid MC tab of the Impact Hybrid Monte Carlo panel is δ . Then the time step used to integrate the slow forces is $\delta/1$, while the time step for medium forces is $\delta/(1 \times 2)$, and that for fast forces is $\delta/(1 \times 2 \times 4)$. Thus, the integration time step decreases as the product of the cumulative RRESPA update frequencies in going from slow to fast forces.

When FMM is not used (this is the more common case), only the Fast forces update frequency affects the calculation. In this case, the Medium and Slow forces are combined and use the global Time step set in the Dynamics tab of the Impact Dynamics panel or in the Hybrid MC tab of the Impact Hybrid Monte Carlo panel. Fast forces use the shorter time step computed by dividing the global Time step by the Fast forces update frequency.

Stop overall motion

When this option is selected (the default), overall rotational and translational motion (drift) of the system is subtracted from the calculation.

Frequency of printing information

This text box selects the frequency with which MD information is written during the simulation. The default is to print information every 5 MD steps. Any integer value greater than zero is allowed.

Collect MD statistics

This option is deselected by default. When it is selected, the MD statistics are collected and are written to the end of the Impact output file. These statistics measure fluctuations of the different energy terms.

Record trajectory

This option is deselected by default. When it is selected, trajectory information is written to the file *jobname.trj* in the Maestro working directory. This information is written in binary format, but can be analyzed using the ANALYSIS task of Impact (which is not, however, supported by Maestro). A trajectory file contains a sequence of snapshots of the coordinates of the system and, if requested, of the velocities as well.

Note: The Impact analysis task must be run using Impact from the command line. See [Chapter 6](#) for a brief overview of command-line Impact. See the *Impact Command Reference Manual* for additional information.

You can view trajectories in Maestro using the Trajectory panel. When the results are incorporated into the project, click the T button in the Aux column of the Project Table for the incorporated entry to open the panel. See [Section 3.5 on page 30](#) for more information.

The following two options are applicable when Record trajectory has been selected:

Frames written every

This text box specifies how often trajectory information is written to the trajectory file. The default is every 5 MD steps. Any integer value greater than zero is allowed.

Sample velocities

This option is on by default. When it is selected, velocity information is written to the trajectory file.

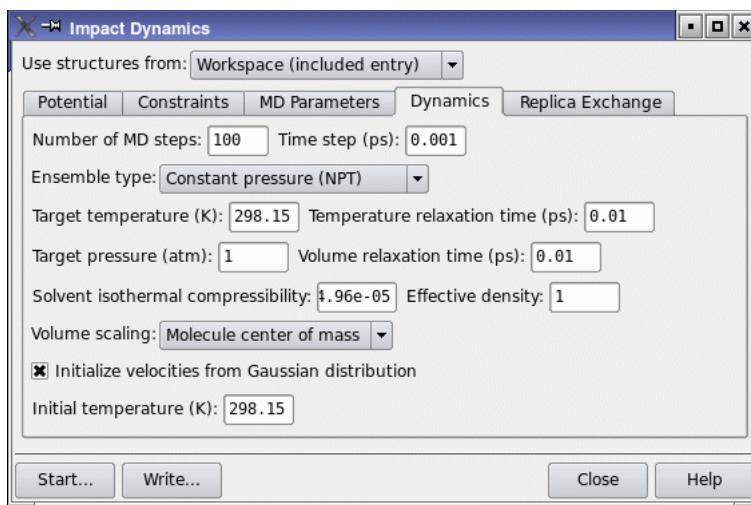


Figure 3.3. *The Dynamics tab of the Impact Dynamics panel.*

3.3 The Dynamics Tab

Use the Dynamics tab to choose the ensemble type, number of steps, time step, and other settings for a molecular dynamics calculation. The major options are described below. The other options in this tab are described under the major option to which they apply.

Number of MD steps

This text box sets the number of MD steps to be used for the simulation. The default setting is 100 steps, but any number greater than zero is allowed.

Time step

This text box sets the time step for the MD simulation. The default value is 0.001 ps, but any value greater than zero is allowed. A somewhat larger value (0.0015 or 0.002) may be suitable if bond lengths are constrained (see [Section 3.1 on page 22](#)) or if the RRESPA integrator is employed (see the MD Parameters tab in [Section 3.2 on page 23](#)).

Ensemble type

Impact offers three choices:

- Constant temperature (NVT)
- Constant energy (NVE)
- Constant pressure (NPT)

Depending on the ensemble chosen, various subsidiary settings become active.

Constant temperature (NVT) (the default)

With this ensemble type, volume and temperature are held constant during the simulation. This selection simulates coupling the system to an external heat bath (with a target temperature that is the same for all molecular species). Two settings become available when this ensemble type is chosen:

- **Target temperature (K)**—This text box sets the target temperature for an NVT or NPT simulation. The actual temperature will fluctuate about the specified value. At each MD step the velocities will be scaled so that the temperature will approach the desired value on a time scale determined by the Temperature relaxation time parameter. The default temperature is 298.15 K; the acceptable range is any value greater than or equal to 0 K.
- **Temperature relaxation time (ps)**—This text box sets the temperature relaxation time in picoseconds for velocity scaling. The default value is 0.01 ps; the acceptable range is any value greater than zero.

Constant energy (NVE)

With this ensemble, no temperature, volume, or pressure scaling is done. However, the total energy may not be conserved if nonbonded interaction cutoffs or too long an MD time step is used. In most cases, failure of energy conservation will lead to an unstable MD simulation. It is recommended that for this ensemble you deselect the nonbonded cutoffs option in the Potential tab, which is selected by default.

Constant pressure (NPT)

For this ensemble, both temperature and pressure are held constant during the simulation. This is accomplished by also coupling the system to a pressure bath using the algorithm of Berendsen et al. (*J. Chem. Phys.* **1984**, 81, **3684**). Seven settings become available when this ensemble type is chosen. Along with Target temperature and Temperature relaxation time, described above, these are:

- **Target pressure (atm)**—This text box specifies the desired pressure in atmospheres. The actual pressure will fluctuate about the desired value. At each MD step the system will be scaled such that the pressure will approach the desired value on a time scale determined by the Volume relaxation time parameter. The default pressure value is 1 atm; the acceptable range is any positive or negative real value.
- **Volume relaxation time (ps)**—This text box sets the volume relaxation time in picoseconds for volume scaling in a constant pressure MD simulation. The default value is 0.01 ps; the acceptable range is any value greater than zero.

- **Solvent isothermal compressibility**—Isothermal compressibility or $k (1/V(dV/dP))$, in units of atm^{-1} is the pressure analogue of the heat capacity and relates to the tendency of the solvent's volume to increase or decrease during pressure fluctuations in the system. The default is the value for water: $4.96 \times 10^{-5} \text{ atm}^{-1}$; the acceptable range is any value greater than zero.
- **Effective density**—This text box specifies the effective density (g/cm^3) of solute molecules. This quantity is used to compute long-range corrections to the pressure during NPT molecular dynamics simulations. The default value is 1.0 g/cm^3 ; the acceptable range is any value greater than zero.
- **Volume scaling**

Select one of two options for volume scaling in a MD simulation:

- **Molecule center of mass**—This method of volume scaling, the default, is best for small molecules and is implemented by scaling the coordinates of the center of mass for each molecular species, relative to the center of the simulation box.
- **Atom based**—This method of volume scaling is best for large molecules and is implemented by uniformly scaling all atomic coordinates relative to the center of the simulation box.

Initialize velocities from Gaussian distribution

When this option, available for all three ensembles, is selected, molecular velocities will be initialized as described, and the Initial temperature text box becomes available.

Initial temperature

When Initialize velocities from Gaussian distribution is selected, this text box specifies the initial temperature for the MD simulation. The default value is 298.15 K; the acceptable range is any value greater than or equal to 0 K.

3.4 The Replica Exchange Tab

Impact supports state-of-the-art temperature replica exchange simulations. These simulations can be run in parallel, using the MPI message passing interface. Use the Replica Exchange tab to set up the number of replicas, the number of steps between exchanges and the temperature settings.

Note: Replica exchange calculations are only supported on Linux-x86 platforms.

The options are described below.

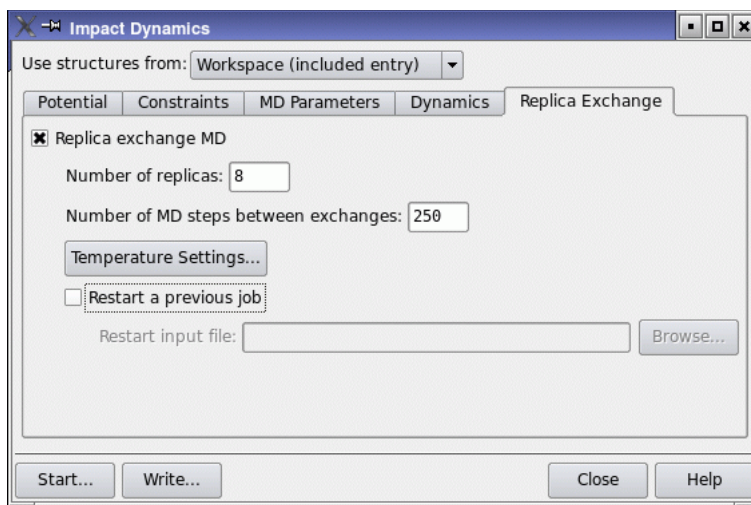


Figure 3.4. The Replica Exchange tab of the Impact Dynamics panel.

Replica exchange MD

Select this option to enable the use of replica exchange. When you do so, the remaining controls in the tab become available.

Number of replicas

Enter the desired number of replicas in this text box. The maximum allowed is 100.

Number of MD steps between exchanges

Enter the number of MD steps to take between exchanges of replicas.

Temperature Settings

This button opens the Temperature Settings dialog box, in which you can set the target temperature for each replica and select the temperature of interest. The dialog box has the following options:

- **Temperature**—Enter the temperature for each replica in these text boxes. The temperatures must be entered in increasing order. The default value for the first temperature is 300 K.
- **Temperature of interest**—Use one of these buttons to select the temperature of interest. Only one temperature can be selected. This is the temperature of the replica whose trajectory will be incorporated into Maestro at the end of the job

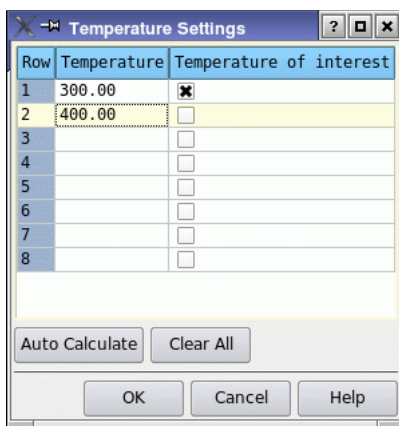


Figure 3.5. The Temperature Settings dialog box.

- **Auto Calculate**—Calculate the temperatures as a geometric series. This button becomes available when the first two temperatures have been entered. These temperatures define the ratio that is used to generate all the other temperatures.
- **Clear All**—Clear all the temperature text boxes.

Restart a previous job

Select this option to restart a calculation using the reference structure output from a previous replica exchange job. You can change parameters except for the temperature settings and the number of replicas.









Restart input file

Enter the name of the reference structure output file you want to use to restart the job, or click Browse and navigate to the output file. The file should normally end in `-out.maegz`.

3.5 Viewing Trajectories

You can play through trajectories, examine individual frames, and export trajectory data in a variety of forms, in the Trajectory panel. To open the Trajectory panel, click the T button in the Aux column of the Project Table for the entry whose trajectory you want to view.

The toolbar in the Trajectory panel contains a standard set of controls for playing through the trajectory frames, which are listed below. The menu bar has one menu, Play, which contains items that correspond to the toolbar buttons.

- | | |
|---|---|
|  | Go to start
Display the first frame. |
|  | Previous
Display the previous frame. |
|  | Play backward
Display the frames in sequence, moving toward the first. |
|  | Stop
Stop playing through the frames. |
|  | Play forward
Display the frames in sequence, moving toward the last. |
|  | Next
Display the next frame. |
|  | Go to end
Display the last frame. |
|  | Loop
Choose an option for repeating the display of the frames. Single direction displays frames in a single direction, then repeats. Oscillate reverses direction each time the beginning or end of the frame set is reached. |

You can control the selection of frames and the speed of play in the Frame control section of the panel.

- The Start and End text boxes define the frames at which play starts and ends. Frames are numbered from 0.
- The Frame slider and frame text box can be used to select the frame to view. The current frame number is displayed in the text box below the slider. The total number of frames is also displayed in a noneditable text box.
- The Step text box sets the number of frames to step when playing through frames. This value does not affect the Frame slider. The frames that are selected for play can be exported as a selection of frames, using the output buttons.
- The Time text boxes display the time for the current frame and the total time for the trajectory. You can enter a time in the text box to select a frame.

The Speed slider sets the speed at which the frames are played.

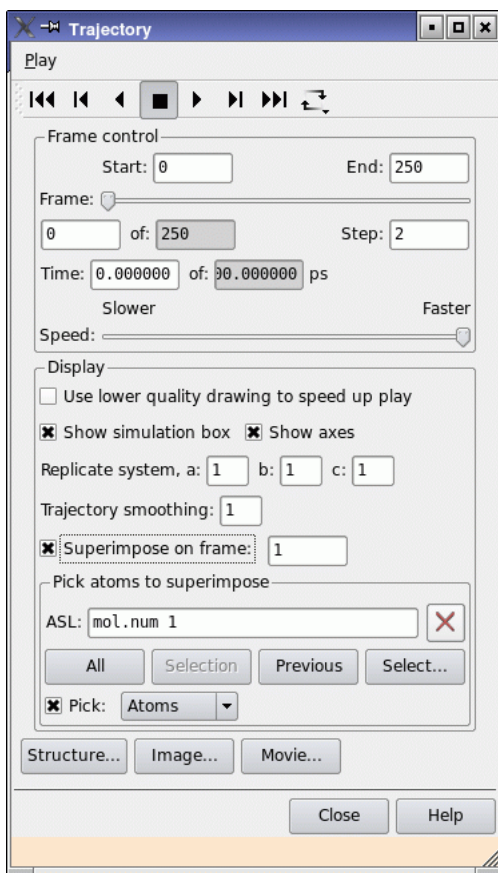


Figure 3.6. The Trajectory panel.

In addition to controlling which frames are displayed and how fast, you can modify the appearance and content of the Workspace during display of frames.

To select the atoms that are visible when frames are displayed, you can use the toolbar buttons that control the atom display:



When you play through the trajectory, the choice that you make for the atoms that are displayed is applied to each frame.

The other controls for what is visible in the Workspace during frame display are:

- **Show simulation box**—Show the edges of the simulation box (in purple).
- **Show axes**—Show the coordinate axes in green.
- **Replicate system**—Enter the number of replicas of the system to display in each of the three directions. This enables you to visualize the movement across the simulation box boundaries. These text boxes are unavailable if there are no periodic boundary conditions.
- **Trajectory smoothing**—Smooth the trajectory by averaging the coordinates over the specified number of frames.
- **Superimpose on frame**—Align the structure in each frame by superimposing a selection of atoms on the corresponding atoms in the frame number given in the text box. Use the **Pick atoms to superimpose** picking controls to make the atom selection. You should consider picking atoms that do not change their position much during the simulation.

The output buttons allow you to export the trajectory data in various forms. You can export individual frames, all frames, or the selection of frames defined by using the **Start**, **End**, and **Step** text boxes. The buttons have the following actions:

- **Structure**—Save structures from the trajectory to a file or create project entries from the structures. Opens the **Export Structure** dialog box, in which you can specify where the structures will go, and which structures to export.
- **Image**—Create an image of the Workspace with the current frame displayed. Opens the **Save Image** panel.
- **Movie**—Save a movie of the trajectory in MPEG format. Opens the **Export Movie** panel, in which you can select the frames to be exported, the speed and the resolution.

Note: Trajectories that are larger than 4GB cannot be viewed in Maestro.

Hybrid Monte Carlo Simulations

You can use the Hybrid Monte Carlo panel to set up and run a Hybrid Monte Carlo (HMC) simulation on the Workspace structure or on a selected entry in the Project Table. HMC simulations achieve relatively efficient sampling by interleaving Monte Carlo moves with a short sequence of molecular-dynamics steps. Because HMC is used mainly as a sampling method, for example, in Liaison binding affinity calculations, the MD steps can use a somewhat larger time step than would normally be advisable. The Metropolis algorithm determines which MD moves should be accepted or rejected. This ensures that the simulation will not go far astray, even if the MD time step would normally lead to a failure of energy conservation. This is why HMC is sometimes called “bad MD but good MC”.

To open the Impact Hybrid Monte Carlo panel, choose Hybrid MC from the Impact submenu of the Maestro Applications menu.

The Impact Hybrid Monte Carlo panel has four tabs:

- Potential
- Constraints
- MD Parameters
- HybridMC

The Potential and Constraints tabs are described in [Chapter 2](#). Additional features of the Constraints tab appear in [Section 3.1 on page 22](#). Features of the MD Parameters tab relevant to both Impact Dynamics and Impact HMC are discussed in [Section 3.2 on page 23](#). The HybridMC tab is discussed below.

When you have set the options in the Impact Hybrid Monte Carlo panel tabs to the desired value, click the Start button to open the Impact Hybrid Monte Carlo - Start dialog box. The standard job start options are displayed, including the Incorporate option menu and the Job options: Name, Host machine, and Username (if different from the username on the local host machine). For a description of these options, see [Section 2.2.3 on page 5](#). The default job name for Impact Hybrid MC jobs is `impact_hmc`.

The input for an Impact Hybrid MC job can be either the contents of the Workspace or a single entry in the Project Table.

Note: *Only one entry from the Maestro Project Table can be displayed and used for each HMC job. If you need to merge two entries, use the Project Table’s Merge option to create a combination entry, and use that as the basis for your simulation.*

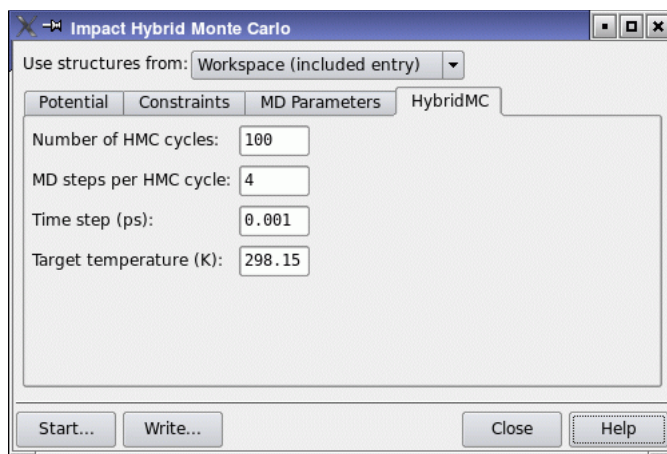


Figure 4.1. The HybridMC tab of the Impact Hybrid Monte Carlo panel.

The HybridMC tab defines the basic settings of the HMC task for an Impact Hybrid Monte Carlo simulation. The selection options are:

Number of HMC cycles

The default number of HMC cycles is 100. The acceptable range is any number greater than zero.

MD steps per HMC cycle

The default number of MD steps per HMC cycle is 4. The acceptable range is any value greater than zero. Liaison simulations use 5 MD steps per HMC cycle.

Time step

This text box sets the MD global time step (in picoseconds) for the simulation. The default value is 0.001 ps. The acceptable range is any value greater than 0 ps. Because energy conservation is less important in HMC simulations, a time step of 0.002 ps or greater may be suitable.

Target temperature

This text box sets the target temperature (in Kelvin) for the HMC simulation. The default initial temperature is 298.15 K. The default target temperature is also 298.15 K. The acceptable range is any value greater than 0 K.

Soak—Add Explicit Water Solvent

Soak surrounds a structure with a box of solvent molecules. You can specify the box size and the solvent type and density. Then Impact adds the solvent molecules, removes any that are too close to the solute, and writes a Maestro-format file for the soaked system.

By default, Soak places 216 water molecules in the smallest permitted solvent box (at least 18.62 Å in each dimension.) The resulting box is not equilibrated due to edge effects. A short minimization is usually sufficient to obtain a fully equilibrated solvated system. It is recommended that constant temperature molecular dynamics, described in [Chapter 3](#), be used for this and any other explicit solvent systems.

To model active sites or water shells around proteins with explicit solvent:

1. Run Soak.
2. Run a short minimization and constant temperature MD equilibration at room temperature.

You can set up a Soak job in the Soak panel. To open the Soak panel, choose Soak from the Impact submenu of the Maestro Applications menu.

When you have set the options in the Soak panel to the desired values, click Start, to open the Start dialog box. In this dialog box you can make job settings and start the job. The Incorporate option menu allows you to append the results to the Project Table or to leave them as a file, which is named *jobname_out.mae*. There is no option to replace existing entries. The default job name for Soak jobs is `impact_soak`. For a description of the Start dialog box options, see [Section 2.2](#) of the *Job Control Guide*.

The input structure for a Soak job can be either the contents of the Workspace or a single entry in the Project Table.

The Soak panel has features common to Impact application panels, such as the Use structures from option menu and the Start, Write, Close, and Help buttons at the foot of the panel. For information on these common features, see [Section 2.2 on page 3](#). The Soak panel also includes a single tab, labeled Soak, with the following options:

Solvent type

The solvent types available are SPC water (Simple Point Charge), TIP4P water, and TIP3P water.

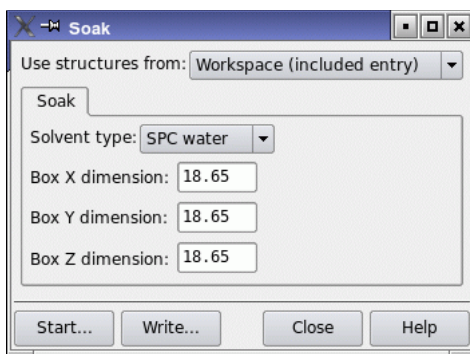


Figure 5.1. The Soak panel.

Box [X,Y,Z] dimensions

Use these three text boxes to specify the required size of the solvent box in angstroms. The minimum (and default) size for any dimension that Maestro will use is 18.65 Å. These values also update the size of the simulation box when periodic boundary conditions are applied. (See the discussion of periodic boundary conditions in [Section 2.4.4 on page 11.](#))

Running Impact from the Command Line

Although you will normally set up jobs using the controls and settings in the Maestro GUI, you can submit Impact jobs either from within Maestro or from the command line. Advantages of running from the command line include:

- The command-line scripts can run all full-featured jobs written using the Impact panels in Maestro, and also allow you to override specific run-time values that are not accessible through the Maestro interface.
- Command-line scripts allow you to run jobs when you want.
- Command-line scripts can be modified and jobs can be re-run without reconfiguring and reloading job settings in Maestro.
- Some job options, such as trajectory file analysis, are available only when you run Impact from the command line.

The `SCHRODINGER` environment variable must be set to run jobs. You can define `SCHRODINGER` as follows:

csh/tcsh: `setenv SCHRODINGER installation-directory`

bash/ksh: `export SCHRODINGER=installation-directory`

Unless otherwise specified, Schrödinger applications and utilities run under a job control system and are automatically run in the background. You need not add an `&` at the end of the commands to have them run and immediately return your command prompt. The `-WAIT` option of the `impact` command forces the shell to wait until the job is finished, so you can embed such commands in other scripts.

6.1 Running Impact From the Command Line

Basic Impact calculations can be run from the command line using the syntax shown below.

```
$SCHRODINGER/impact [options] [-i] input-file
```

To run `impact`, you must specify the input file, *input-file*. If *input-file* does not end in `.inp`, Impact looks first for *input-file* as specified. If that file doesn't exist, it then looks for *input-file.inp*. If `-i` is omitted, then *input-file* **must** end in `.inp` and must be the last argument in

the command line. If `-i` is included, the input file specification can be placed anywhere on the command line.

The options that you can specify when initiating jobs from the command line are described in [Table 6.1](#). The standard Job Control options and the options `-WAIT` and `-LOCAL`, described in [Table 2.1](#) and [Table 2.2](#) of the *Job Control Guide*, are also supported. To view the usage summary information, define the `SCHRODINGER` environment variable and enter `$SCHRODINGER/impact -h` in a terminal window.

Table 6.1. *Impact command options*

Option	Description
<code>-h</code>	Print usage summary and exit
<code>-v</code>	Print version number of startup script and exit
<code>-o output-file</code>	File for writing output and log messages. If this option is omitted, Impact names the log file <i>jobname.log</i> , where <i>jobname</i> is taken from the Impact input file name.
<code>-s size</code>	Use specific “size” version of the Impact executable. Acceptable values for <i>size</i> are <i>medium</i> or <i>huge</i> . If omitted, <i>medium</i> is assumed in most cases; it is valid for up to 8000 atoms or 8000 bonds. The <i>huge</i> option accommodates up to 40000 atoms or 40000 bonds.

Note: The default molecular mechanics force field for Basic Impact applications is the OPLS_2005 version of OPLS-AA. OPLS_2001 is also available. OPLS_2001 and OPLS_2005 are designed to work with automatic atom-typing, and are incompatible with template mode. If you attempt to write a template file (Impact command `WRITE TEMPLATE`) while using OPLS_2001, an error message is displayed to remind you that this command can only be used with OPLS1999 or OPLS2000 force fields. To use one of these older force fields, add a line to your input file before the `CREATE` task, for example:

```
SET FFIELD OPLS1999
```

For distributed processing, the `run_jobs.pl` script can be used. (Distributed processing for Basic Impact calculations is not available from the GUI.)

Impact jobs run under the Job Control facility. You can use the `$SCHRODINGER/jobcontrol` command to monitor and manage jobs. For more information on this command and the Job Control facility, see the [Job Control Guide](#).

6.2 File Name Conventions

A typical Impact job has one command-script file (*jobname.inp*), one or more structure files (*jobname.mae*, *jobname.pdb*, or *jobname.sdf*), and after execution, several output files (e.g., *jobname_out.mae* for structure files and *jobname.out* for textual data).

If a file already has the name of an output file, in many cases Impact renames the old file with a numerical extension (*filename.out.01*, *filename.out.02*, and so on) for archival purposes. The new job's output is then written to the base name (*filename.out*). If you do not need the old files, you can remove them.

Some files, such as *jobname.log* files, are newly written each time Impact runs a calculation. Likewise, old *jobname_pv.mae* files are overwritten. For Impact minimization jobs, the *jobname_out.mae* structure file is *not* incremented.

Table 6.2 contains descriptions of the various file types. For more information, see the Maestro online help or the [Impact Command Reference Manual](#).

Table 6.2. Liaison file extensions

Extension	Description
.inp	Impact input file or script. Impact input files are formatted plain-text files written in the Impact input file language, DICE. Maestro creates Impact input files before job submission, or you can create or edit them manually with a text editor.
.mae	A Maestro format structure file, a plain-text file written by Maestro containing atom, bond, and other information for one or more molecules.
.log	An Impact log file. If specified, a .log file captures standard output and standard error messages in text form. This file is overwritten during subsequent runs.
.out	An Impact output file containing information similar to that found in log files (no standard error). Output files are appended with numerical extensions when the input file is run again. Up to 99 output files are retained.
.01, .02, etc.	A file containing results from previous Impact calculations run from the corresponding <i>jobname.inp</i> file.
_out.mae	An Impact output structure file written in the Maestro file format. Liaison and some Impact jobs do not write *_out.mae output structure files.

Getting Help

Schrödinger software is distributed with documentation in PDF format. If the documentation is not installed in `$SCHRODINGER/docs` on a computer that you have access to, you should install it or ask your system administrator to install it.

For help installing and setting up licenses for Schrödinger software and installing documentation, see the *Installation Guide*. For information on running jobs, see the *Job Control Guide*.

Maestro has automatic, context-sensitive help (Auto-Help and Balloon Help, or tooltips), and an online help system. To get help, follow the steps below.

- Check the Auto-Help text box, which is located at the foot of the main window. If help is available for the task you are performing, it is automatically displayed there. Auto-Help contains a single line of information. For more detailed information, use the online help.
- If you want information about a GUI element, such as a button or option, there may be Balloon Help for the item. Pause the cursor over the element. If the Balloon Help does not appear, check that Show Balloon Help is selected in the Maestro menu of the main window. If there is Balloon Help for the element, it appears within a few seconds.
- For information about a panel or the tab that is displayed in a panel, click the Help button in the panel, or press F1. The help topic is displayed in your browser.
- For other information in the online help, open the default help topic by choosing Online Help from the Help menu on the main menu bar or by pressing CTRL+H. This topic is displayed in your browser. You can navigate to topics in the navigation bar.

The Help menu also provides access to the manuals (including a full text search), the FAQ pages, the New Features pages, and several other topics.

If you do not find the information you need in the Maestro help system, check the following sources:

- *Maestro User Manual*, for detailed information on using Maestro
- *Maestro Command Reference Manual*, for information on Maestro commands
- *Maestro Overview*, for an overview of the main features of Maestro
- *Maestro Tutorial*, for a tutorial introduction to basic Maestro features
- *Impact Command Reference Manual*, for detailed information on Impact commands
- Impact Frequently Asked Questions pages, at https://www.schrodinger.com/Impact_FAQ.html

- Known Issues pages, available on the [Support Center](#).

The manuals are also available in PDF format from the Schrödinger [Support Center](#). Local copies of the FAQs and Known Issues pages can be viewed by opening the file `Suite_2009_Index.html`, which is in the `docs` directory of the software installation, and following the links to the relevant index pages.

Information on available scripts can be found on the [Script Center](#). Information on available software updates can be obtained by choosing Check for Updates from the Maestro menu.

If you have questions that are not answered from any of the above sources, contact Schrödinger using the information below.

E-mail: help@schrodinger.com
USPS: Schrödinger, 101 SW Main Street, Suite 1300, Portland, OR 97204
Phone: (503) 299-1150
Fax: (503) 299-4532
WWW: <http://www.schrodinger.com>
FTP: <ftp://ftp.schrodinger.com>

Generally, e-mail correspondence is best because you can send machine output, if necessary. When sending e-mail messages, please include the following information:

- All relevant user input and machine output
- Impact purchaser (company, research institution, or individual)
- Primary Impact user
- Computer platform type
- Operating system with version number
- Impact version number
- Maestro version number
- mmshare version number

On UNIX you can obtain the machine and system information listed above by entering the following command at a shell prompt:

```
$SCHRODINGER/utilities/postmortem
```

This command generates a file named `username-host-schrodinger.tar.gz`, which you should send to help@schrodinger.com. If you have a job that failed, enter the following command:

```
$SCHRODINGER/utilities/postmortem jobid
```

where *jobid* is the job ID of the failed job, which you can find in the Monitor panel. This command archives job information as well as the machine and system information, and

includes input and output files (but not structure files). If you have sensitive data in the job launch directory, you should move those files to another location first. The archive is named `jobid-archive.tar.gz`, and should be sent to help@schrodinger.com instead.

If Maestro fails, an error report that contains the relevant information is written to the current working directory. The report is named `maestro_error.txt`, and should be sent to help@schrodinger.com. A message giving the location of this file is written to the terminal window.

More information on the `postmortem` command can be found in [Appendix A](#) of the *Job Control Guide*.

On Windows, machine and system information is stored on your desktop in the file `schrodinger_machid.txt`. If you have installed software versions for more than one release, there will be multiple copies of this file, named `schrodinger_machid-N.txt`, where *N* is a number. In this case you should check that you send the correct version of the file (which will usually be the latest version).

If Maestro fails to start, send email to help@schrodinger.com describing the circumstances, and attach the file `maestro_error.txt`. If Maestro fails after startup, attach this file and the file `maestro.EXE.dmp`. These files can be found in the following directory:

```
%USERPROFILE%\Local Settings\Application Data\Schrodinger\appcrash
```


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